HPCAT NEWSLETTER

August 2006 **Volume 1, Number 1**

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Introduction by Guoyin Shen

HPCAT has been running a combination of construction, commissioning, and user operation since 2002. With a multidisciplinary approach and multi-institution collaborations, the high-pressure program at HPCAT has been enabling myriad scientific breakthroughs in high-pressure researches. Through collaboration with other APS sectors and other facilities, an array of various x-ray measurements has been integrated with high pressure instrumentation at HPCAT, from novel synchrotron spectroscopic techniques to dramatically improved x-ray micro-diffraction with an accuracy and sophistication that rival ambient structural determinations. In its 7th year from the formation of HPCAT, many proposed goals have been realized with many successes beyond our initial expectations. The on-board HPCAT staff has been putting tremendous efforts in every stage of developments, from design, procurement, installation, commissioning, and operation, to sample preparation, data analysis, safety procedures, and science results. Together with member users and general users of HPCAT, great progresses in the high pressure program have been made as shown by the quality and quantity of its publications. It is a great privilege to be part of this wonderful group and to witness the daily excitements at HPCAT. As we moves into mature operation with unique capabilities for exploring the frontiers in high pressure science, we start this HPCAT Newsletter covering exciting developments and other news items.

For general information about HPCAT, our web-page is always a good start. Further information can be obtained by attending HPCAT Committee (HPC) meetings and by directly contacting HPCAT staff.

Science Highlights by Haozhe Liu

Iron-rich silicates in ultralow-velocity zones

With the discovery of the post-perovskite (ppv) phase in $MgSiO_3$, and subsequent results indicating ppv can incorporate a considerable amount of the Fe, a group led by Wendy Mao shows how Fe would affect the properties of ppv and whether experimental results on Fe-rich ppv would match seismic observations near the core-mantle boundary (CMB). Together with the results from nuclear resonant x-ray scattering performed at sector 3, aggregate sound velocities for a ppv composed of 40% of the Fe endmember, i.e. $(Mg_{0.6}Fe_{0.4})SiO_3$, were obtained. Fe-rich ppv can reproduce the dramatic depression in seismic velocities observed in ultralow velocity

Members' Websites:

Carnegie

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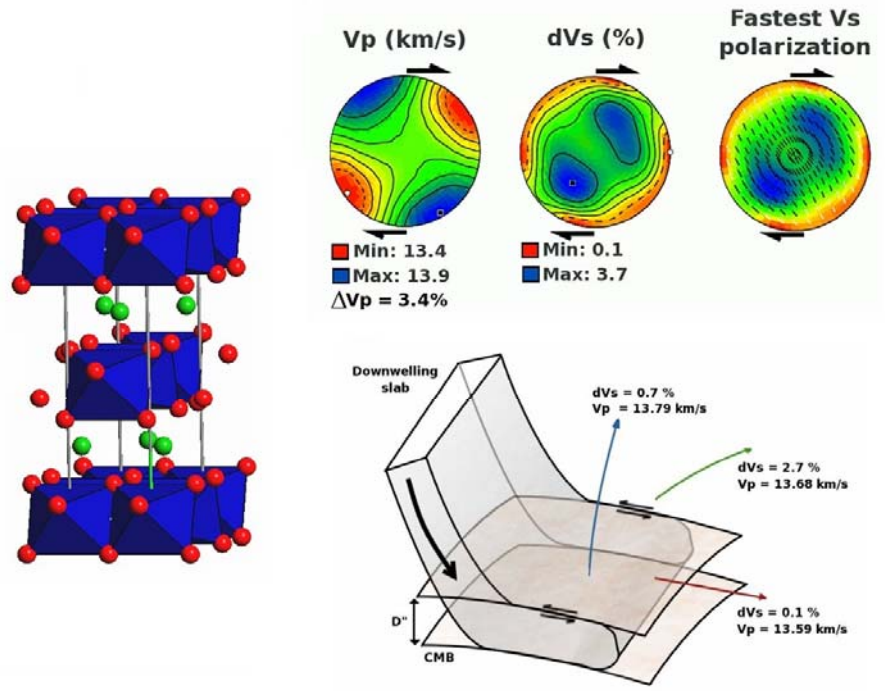
zones (ULVZ)—i.e. thin 5-40 km thick patches just above the CMB where compressional and shear wave velocities are lowered by ~10% and 30% respectively relative to the results from seismic observations—providing an alternative explanation for the origin of ULVZ. Although further studies are still needed, these results provide an exciting new direction into the dominating role Fe-rich ppv may play at the CMB, where the silicate mantle is in contact with the Fe-rich, liquid outer core.

Full article: Mao, W.L., Mao, H.K., Sturhahn, W., Zhao, J., Prakapenka, V.B., Shu, J., Fei, Y., and Hemley, R.J., 2006, Iron-rich post-perovskite and the origin of ultralow-velocity zones: ***Science***, v. 312, p.564-565.

Plastic Behavior of Post-Perovskite Deep in the Earth's Interior

Under the pressures of the core-mantle boundary (2900km below the surface), the main constituent of the deep mantle, silicate perovskite, undergoes a phase transition to a post-perovskite phase whose mechanical properties remain unknown. A recent study published in Science shows the development lattice preferred orientations in an analogue of silicate post-perovskite plastically deformed above 100 GPa. The experiments were carried out inside a diamond anvil pressure cell and the measurements performed using x-ray diffraction at the HPCAT. It is found that (100) and (110) slip dominate the plastic deformation of post-perovskite. The contribution of post-perovskite to shear wave splitting should range from 0.1 to 3.1% for waves traveling in the plane of shear. In agreement with recent seismic observations of tilted transverse anisotropy in D", for silicate

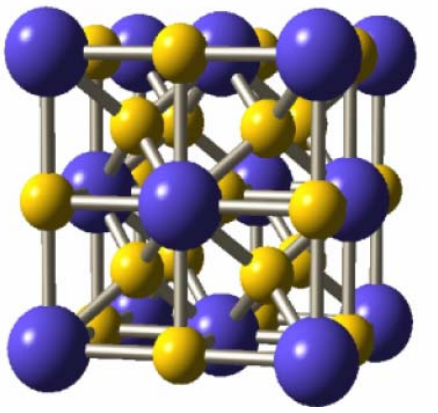


Contribution of silicate p-Pv to seismic anisotropy in D" after 20% deformation in shear

post-perovskite the polarization anisotropy is usually inclined by about 45 degrees compared with the plane of shear. These results underline the importance of high-pressure experimentation in assessing plasticity and seismic anisotropy in the deep Earth.

Full article: Sebastien Merkel, Atsushi Kubo, Lowell Miyagi, Sergio Speziale, Thomas S. Duffy, Ho-kwang Mao, Hans-Rudolf Wenk, Plastic Deformation of $MgGeO_3$ Post-Perovskite at Lower Mantle Pressures, ***Science***, 311, 644, 2006.

Structure and Stability of Low-Z Ionic Solids at High Pressure.



Pressure-induced phase transitions in a class of highly ionic low-Z compounds with simple structures have been recently studied using synchrotron x-ray diffraction and spectroscopy in diamond anvil cells at HPCAT, together with electronic structure calculations. Results for Li_3N and Li_2O reveal some original and unexpected properties in this class of closed-shell materials and in their hydrogen-containing analogs NH_3 and H_2O. Li_3N is found to have a hexagonal to cubic structural transition at 40 GPa, accompanied by a volume collapse and electronic band-gap widening. The cubic phase is stable to at least 200 GPa and, over this pressure range, the band gap continues to widen and the material retains its closed-shell (N^{3-}, isovalent to neon) ionic character, i.e., pressure is driving the system to a more strongly ionic state! Cubic-Li_3N follows the same trend in compressibility as neon and both are predicted to metallize at extremely high (multi-TPa) pressure. Li_2O, which is structurally and electronically similar to high pressure ice, undergoes a cubic-orthorhombic transition at 50 GPa, with a 100% increase in bulk modulus. Considered with the known behavior of alkali sulfides, the results for Li_2O indicate a systematic high-pressure behavior of all alkali chalcogenides, perhaps even including non-molecular ice at ultra-high pressure.

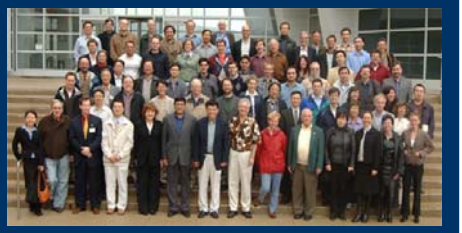
Full articles:1. A. Lazicki, B. Maddox, W. Evans, C. S. Yoo, A. K. McMahan, W. E. Pickett, R. T. Scalettar, M. Y. Hu, and P. Chow, New Cubic Phase of Lithium Nitride to 200 GPa: high ionic stability of N^{3-} ions, ***Phys. Rev. Lett.*** 95, 165503 (2005)

2. A. K. Lazicki, C. S. Yoo, W.J. Evans, W.E. Pickett, and R.T. Scalettar, Pressure-Induced Antifluorite-to-Anticotunnite Phase Transition in Lithium Oxide, ***Phys. Rev. B***. 73, 184120 (2006).

News and Updates by Veronica O'Connor

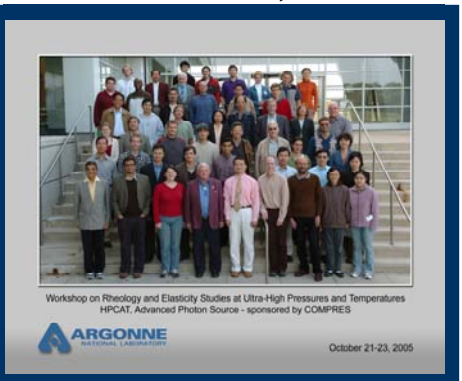
HPCAT Staff…

Row 1 from left to right: Arunkumar Bommannavar, Yue Meng, Paul Chow, Veronica O'Connor
Row 2 from left to right: Yang Ding, Eric Rod, Michael Hu, Guoyin Shen
Row 3 from left to right: Hanns-Peter Liermann, Stanislav Sinogeikin, Haozhe Liu, Kevin Westman
Row 4 from left to right: Ho-kwang (Dave) Mao, Wenge Yang



- The Workshop on Synergy of 21st Century High-Pressure Science and Technology was held April 29 through May 1, 2006 at the Advanced Photon Source at Argonne National Laboratory. The workshop provided a forum to review the status of U.S. High-pressure research and identified future grand challenges. The group discussed the great scientific potential in establishing a next-generation "synergetic consortium" that would integrate state-of-the-art high-pressure techniques, facilities, and probes, and make them readily accessible to multidisciplinary high-pressure scientists. The consortium would enable high-pressure specialists and non-specialists alike to focus on specific scientific goals which were previously hindered due to technical limitations.

The workshop was jointly sponsored by the Consortium for Materials Properties Research in Earth Sciences (COMPRES), Carnegie/DOE Alliance Center (CDAC), and



the High-Pressure Collaborative Access Team (HPCAT). Attendees came from both academic institutions and the National Labs around the country.

• The workshop on "Rheology and Elasticity Studies at Ultra-High Pressures and Temperatures" held on Oct 21-23, 2005 at APS, organized by Haozhe Liu, Hans-Rudolf Wenk, and Thomas S. Duffy has provided an opportunity to assemble more than 50 scientists from 6 countries. Experts in diamond anvil cell design, large volume high-pressure apparatus, and data analysis defined the current state of ultra-high pressure deformation studies and explored initiatives to push the technological frontier. The proceedings were recently published in *Journal of Physics: Condensed Matter, 18(25), 2006*.

The workshop was jointly sponsored by the Consortium for Materials Properties Research in Earth Sciences (COMPRES), and the High-Pressure Collaborative Access Team (HPCAT).

• The International Balzan Foundation has awarded Russell J. Hemley and Ho-kwang (Dave) Mao of the Geophysical Laboratory, Carnegie Institution of Washington the Balzan Prize for 2005 in Mineral Physics. They have developed techniques which allow them to study the behavior of a wide range of materials, such as hydrogen. Their results have deep implications for our understanding of nature.


Verteilen statt sparen: Bundesrat Couchepin mit den Preisträgern Russell J. Hemley und He-kwang Mao (ganz rechts) im Nationalratssaal


Shaun Doran


Alaina Beres

• THE NEW FACES AT HPCAT are those of project manager Guoyin Shen and beamline scientists Wenge Yang and Stanislav (Stas) Sinogeikin. Welcome!

• Joining HPCAT are summer interns Shaun Doran and Alaina Beres. Also visiting HPCAT are student Tony Shen, and from the Chinese Academy of Sciences Jing Liu and Hui Li.

Tony Shen

• Former project manager Daniel Hausermann assumed a position in Australia; former staff Maddury Somayazulu is now at Geophysical Laboratory.

• The HPCAT Technical Advisory Committee (TAC) was formed in May 2006. The members include Chi-Chang Kao, Martin Kunz, Mark Rivers, Wolfgang Sturhahn, and De-Ming Shu. The Committee met with HPCAT people on June 28, 2006.

• Haozhe Liu headed the newly formed Powder Diffraction group meeting held July 13 at the Advanced Photon Source. Speakers included Wenge Yang (HPCAT) and John Parise. The next meeting will be September 14, headed by Yue Meng (HPCAT). For more information, see: http://www.hpcat.aps.anl.gov/powder_group/monthly_meeting.htm

• Michael Hu gave an invited talk at The Fourth Nassau Mössbauer Symposium 2006 Jan. 13 - 14, 2006, Nassau Community College, Garden City, NY entitled, "Nuclear forward scattering and X-ray emission spectroscopy study of BiFeO3 under high pressures."

• Guoyin Shen attended the High Pressure Gordon Conference in June 25-28, 2006, and gave an invited talk on amorphous materials under high pressure.

• Congratulations Haozhe Liu on your cover design for last year's Carnegie Christmas card! If you haven't seen it yet, visit:

http://www.hpcat.aps.anl.gov/Hliu/2006CIW-Card2.pdf

• Michael and Lulu Hu had their first baby girl last August. Her name is Jiadi. They are still waiting for her to tell what she meant by "dada, nana, tata, mama, baba." Well, the last two have become clearer now.

HPCAT Beamlines

• **Notices for the coming winter cycle of 2006-3**

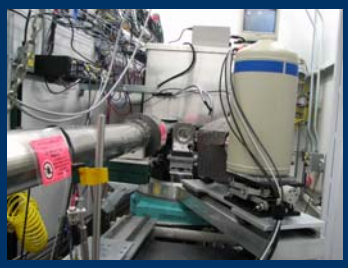
In the run cycle of 2006-3, October-December, on-line laser heating capability will not be available in 16-ID-B, due to major re-configuration in the station. The new laser heating system will be operational in the cycle of 2007-1, January-April.

The 16BM beamline at HPCAT will be open to general users starting the run cycle of 2006-3. The bending magnet beamline is equipped with micro-diffraction facilities, and is currently operational in energy dispersive mode. A monochromator will be installed in early 2007 for angle dispersive diffraction and x-ray absorption spectroscopies.

• Since the first white beam in August, 2005, the 16BM-D station has been under construction and commissioning. The commissioning of a micro-diffractometer has been successful with participation of HPCAT members and the single crystal project led by Przemek Dera. The station is now ready for general users.

• The setup at 16BM-B has been completely reconfigured due to the delivery pipe through the station. The new setup is under commissioning with member users and will be open to general users in the winter cycle of 2006.

• An x-ray beam diagnostic system has been installed in 16ID-A. The system successfully enables the energy calibration, beam position measurement, and x-ray flux monitoring for branch line to 16ID-B.



• In March 2005, HPCAT installed an x-ray emission spectroscopy (XES) spectrometer in 16ID-D which allows us to separate IXS and XES experiment setups. It improves the capability and our efficiency to run XES experiments.

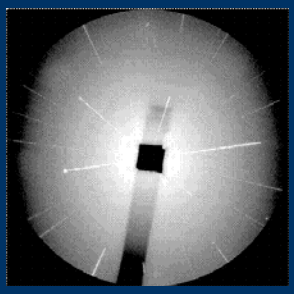
• The compound focusing has been commissioned in 16ID-D. The resulting focus spot is 11x22 microns. The project is still in progress in order to reach optimum focus size and have accurate efficiency measurement.

• A dedicated table for laser heating system in 16ID-B is being designed and to be installed in fall 2006. The existing table will be reconfigured for general purpose diffraction, including those at low temperatures with cryostats.

• The bimorph mirrors in 16ID-B has been replaced by a pair of 200 mm long KB mirrors. A beam size of 5x5 microns can be routinely reached with the new KB mirrors.

• The laser heating optics in 16ID-B has been reconfigured for improved mechanical stability and user-friendly operation.

• An artificial channel-cut monochromator is under construction to be installed in 16BM-C. The silicon-111 monochromator will deliver mono beams to 16BM-D with energy range of 6-56 keV at a vertical beam size of 2 mm. At a reduced beam size, the energy could go higher. The monochromator is equipped with a fixed exit, so there is no beam position change with energy tuning.



• An on-line Raman system has been constructed and tested. The system has been successfully used with cryostats and external heated diamond cells.

• The Raman system has been fine-tuned and works well.

• Beryllium is now widely used in HPCAT experiments. A safety procedure has been established for handling beryllium gasket. For more information, see:
http://www.hpcat.aps.anl.gov/Besafety.htm

• Oxygen monitors have been installed in all four experimental

stations - a safety item for cryogenic and other experiments.

Member and User Highlights

The Advanced Photon Source Users Organization (APSUO) announced that Wendy L. Mao was the recipient of the 2006 "Rosalind Franklin Young Investigator Award." Wendy L. Mao has made contributions to an exceptionally broad range of topics, from the structure of graphite under pressure, to the properties of iron-rich materials at the boundary between the Earth's core and mantle, to the synthesis and characterization of a new family of hydrogen storage materials based on molecular compounds. Wendy received this award on May 3 at the 2006 APS Users Meeting, where she presented her work.

PhD Students from the past year:

Kevin Hope, University of Alabama, Birmingham

Wendy Mao, University of Chicago

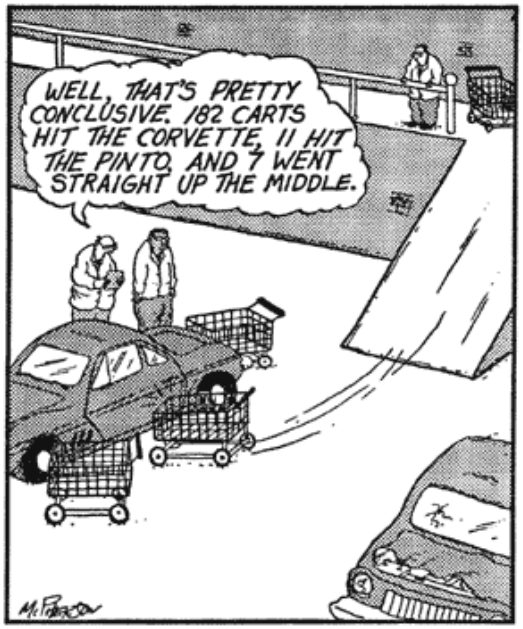
Jenny Pehl, University of California, Berkeley

Wei Qiu, University of Alabama, Birmingham

Nenad Velisavljevic, University of Alabama, Birmingham

HPCAT members include
Carnegie Institution of Washington (Ho-Kwang (David) Mao),
Lawrence Livermore National Laboratory (Choong-Shik Yoo),
University of Hawaii (Murli H. Manghnani),
University of Nevada at Las Vegas (Malcolm Nicol), and
Carnegie / DOE Alliance Center (Russell J. Hemley).

Funnies!!!



Researchers at MIT prove that rolling shopping carts will almost invariably hit the most expensive car in their vicinity.

Laugh, it feels good

Upcoming Events/Deadlines

August 18-20, 2006: HPCAT SECTOR 16-ID-B will be hosting the Eighth National School on Neutron and X-ray Scattering

Directors: Raymond Osborn and Dean Haeffner

September 8-9, 2006: HPCAT Retreat at Starved Rock
www.starvedrocklodge.com

October 3, 2006: Beginning of Run 2006-3

November 3, 2006: General and Partner User proposal deadline, Run 2007-1

Acknowledgment: HPCAT would like to thank Summer Intern, Alaina Beres for her endeavors in creating and compiling the information within this newsletter.